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APPLICATION NO.	FILING DATE	FIRST NAMED INVENTOR	ATTORNEY DOCKET NO.	CONFIRMATION NO.
10/723,594	11/26/2003	Yuan-Ping Pang	07039-161002	7578

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FISH & RICHARDSON P.C.  
PO BOX 1022  
MINNEAPOLIS, MN 55440-1022

EXAMINER
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NEGIN, RUSSELL SCOTT

ART UNIT	PAPER NUMBER
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1631

NOTIFICATION DATE	DELIVERY MODE
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06/12/2009

ELECTRONIC

**Please find below and/or attached an Office communication concerning this application or proceeding.**

The time period for reply, if any, is set in the attached communication.

Notice of the Office communication was sent electronically on above-indicated "Notification Date" to the following e-mail address(es):

PATDOCTC@fr.com

<b>Office Action Summary</b>	<b>Application No.</b> 10/723,594	<b>Applicant(s)</b> PANG, YUAN-PING	
	<b>Examiner</b> RUSSELL S. NEGIN	<b>Art Unit</b> 1631	

-- The MAILING DATE of this communication appears on the cover sheet with the correspondence address --

### Period for Reply

A SHORTENED STATUTORY PERIOD FOR REPLY IS SET TO EXPIRE 3 MONTH(S) OR THIRTY (30) DAYS, WHICHEVER IS LONGER, FROM THE MAILING DATE OF THIS COMMUNICATION.

- Extensions of time may be available under the provisions of 37 CFR 1.136(a). In no event, however, may a reply be timely filed after SIX (6) MONTHS from the mailing date of this communication.
- If NO period for reply is specified above, the maximum statutory period will apply and will expire SIX (6) MONTHS from the mailing date of this communication.
- Failure to reply within the set or extended period for reply will, by statute, cause the application to become ABANDONED (35 U.S.C. § 133). Any reply received by the Office later than three months after the mailing date of this communication, even if timely filed, may reduce any earned patent term adjustment. See 37 CFR 1.704(b).

### Status

- 1) ☒ Responsive to communication(s) filed on 23 March 2009.
- 2a) ☒ This action is **FINAL**.                      2b) ☐ This action is non-final.
- 3) ☐ Since this application is in condition for allowance except for formal matters, prosecution as to the merits is closed in accordance with the practice under *Ex parte Quayle*, 1935 C.D. 11, 453 O.G. 213.

### Disposition of Claims

- 4) ☒ Claim(s) 37-72 is/are pending in the application.
- 4a) Of the above claim(s) \_\_\_\_\_ is/are withdrawn from consideration.
- 5) ☐ Claim(s) \_\_\_\_\_ is/are allowed.
- 6) ☒ Claim(s) 37-72 is/are rejected.
- 7) ☐ Claim(s) \_\_\_\_\_ is/are objected to.
- 8) ☐ Claim(s) \_\_\_\_\_ are subject to restriction and/or election requirement.

### Application Papers

- 9) ☐ The specification is objected to by the Examiner.
- 10) ☐ The drawing(s) filed on \_\_\_\_\_ is/are: a) ☐ accepted or b) ☐ objected to by the Examiner.  
Applicant may not request that any objection to the drawing(s) be held in abeyance. See 37 CFR 1.85(a).  
Replacement drawing sheet(s) including the correction is required if the drawing(s) is objected to. See 37 CFR 1.121(d).
- 11) ☐ The oath or declaration is objected to by the Examiner. Note the attached Office Action or form PTO-152.

### Priority under 35 U.S.C. § 119

- 12) ☐ Acknowledgment is made of a claim for foreign priority under 35 U.S.C. § 119(a)-(d) or (f).
- a) ☐ All    b) ☐ Some \*    c) ☐ None of:
1. ☐ Certified copies of the priority documents have been received.
  2. ☐ Certified copies of the priority documents have been received in Application No. \_\_\_\_\_.
  3. ☐ Copies of the certified copies of the priority documents have been received in this National Stage application from the International Bureau (PCT Rule 17.2(a)).

\* See the attached detailed Office action for a list of the certified copies not received.

### Attachment(s)

- |  |   |
|--|---|
| 1) <input checked="" type="checkbox"/> Notice of References Cited (PTO-892)          | 4) <input type="checkbox"/> Interview Summary (PTO-413)           |
| 2) <input type="checkbox"/> Notice of Draftsperson's Patent Drawing Review (PTO-948) | Paper No(s)/Mail Date. _____                                      |
| 3) <input type="checkbox"/> Information Disclosure Statement(s) (PTO/SB/08)          | 5) <input type="checkbox"/> Notice of Informal Patent Application |
| Paper No(s)/Mail Date _____  | 6) <input type="checkbox"/> Other: _____                          |

## **DETAILED ACTION**

### ***Comments***

Applicants' amendments and request for reconsideration in the communication filed on 23 March 2009 are acknowledged and the amendments are entered.

Claims 37-72 are pending and examined in the instant application.

### ***Withdrawn Objections/Rejections***

ALL of the rejections and objections are withdrawn in view of amendments filed by applicant on 23 March 2009. ALL of the rejections applied in the instant Office action are NEWLY applied and necessitated by applicant's amendments.

### ***Priority***

In view of amendments filed to the instant set of claims, the benefit date of the instant set of claims is now 18 June 1999.

### ***Claim Rejections - 35 USC § 101***

The following rejection is newly applied and necessitated by applicant's amendment:

35 U.S.C. 101 reads as follows:

Whoever invents or discovers any new and useful process, machine, manufacture, or composition of matter, or any new and useful improvement thereof, may obtain a patent therefor, subject to the conditions and requirements of this title.

Claims 55-72 are rejected under 35 U.S.C. 101 because the claimed invention is directed to non-statutory subject matter.

Claims 55-72 are drawn to a computer readable computer program; computer programs, per se, are not statutory.

Response to Arguments:

Applicant's arguments filed 23 March 2009 have been fully considered but they are not persuasive.

Applicant argues that the amendments to the claims overcome the rejection of record. This argument is not persuasive because, as discussed above, computer programs, not limited to be embodied on a physical medium, are not statutory. It is noted that claim 55 recites a "computer readable computer program in tangible form;" however, it is unclear what is intended by a program "in tangible" form (see below). The claims do not limit the program to be carried on, or reside on, etc. any physical medium, therefore the claim is interpreted to be directed to a computer program, per se. It is noted that a computer **storage** medium is usually interpreted to be a physical medium, thus a computer storage medium comprising an executable program is usually interpreted to be directed to statutory subject matter. Applicant is reminded that any amendment must be fully supported and enabled by the originally filed disclosure.

***Claim Rejections - 35 USC § 112***

The following rejections are NEWLY applied and necessitated by applicant's amendment:

The following is a quotation of the second paragraph of 35 U.S.C. 112:

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The specification shall conclude with one or more claims particularly pointing out and distinctly claiming the subject matter which the applicant regards as his invention.

## INDEFINITENESS

Claims 55-72 are rejected under 35 U.S.C. 112, second paragraph, as being indefinite for failing to particularly point out and distinctly claim the subject matter which applicant regards as the invention.

While claims 55-72 recite a "computer program in tangible form," the term "tangible form" is not defined or exemplified in the specification. As a result, it is indefinite as to what this "tangible form" comprises (i.e. a computer storage medium). It is recommended that applicant clarify the intended meaning and the metes and bounds of the term "tangible form."

## WRITTEN DESCRIPTION

The following is a quotation of the first paragraph of 35 U.S.C. 112:

The specification shall contain a written description of the invention, and of the manner and process of making and using it, in such full, clear, concise, and exact terms as to enable any person skilled in the art to which it pertains, or with which it is most nearly connected, to make and use the same and shall set forth the best mode contemplated by the inventor of carrying out his invention.

Claims 55-72 are rejected under 35 U.S.C. 112, first paragraph, as failing to comply with the written description requirement. The claim(s) contains subject matter which was not described in the specification in such a way as to reasonably convey to one skilled in the relevant art that the inventor(s), at the time the application was filed, had possession of the claimed invention.

The specification and drawings are silent with regard to disclosing the limitation of a "computer program in tangible form." While page 8 of the specification discloses

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the computer simulation program AMBER, there is no teaching that this program is, in itself tangible, nor that it resides on a tangible medium. In the absence of such a teaching in the specification, drawings, and original claims, this limitation of a tangible media comprising a program constitutes NEW MATTER.

### ***Claim Rejections - 35 USC § 103***

The following is a quotation of 35 U.S.C. 103(a) which forms the basis for all obviousness rejections set forth in this Office action:

(a) A patent may not be obtained though the invention is not identically disclosed or described as set forth in section 102 of this title, if the differences between the subject matter sought to be patented and the prior art are such that the subject matter as a whole would have been obvious at the time the invention was made to a person having ordinary skill in the art to which said subject matter pertains. Patentability shall not be negated by the manner in which the invention was made.

The following rejection is newly applied and necessitated by applicant's amendments:

#### 35 U.S.C. 103 Rejection #1:

Claims 37-41, 44-47, 52-59, 62-65, and 68-72 are rejected under 35 U.S.C. 103(a) as being unpatentable over Clemmer et al. [Nature, volume 372, 1994, pages 248-250] as evidenced by "Niobium element facts" [obtained online 31 May 2009, referred to in the Office action as 'Niobium'] as evidenced by Schlatholter et al. [J. Phys. B.: At. Mol. Opt. Phys. Volume 31, 1998, pages 1321-1331] in view of Stote et al. [Proteins: Structure, Function, and Genetics; 1995, volume 23, pages 12-31].

Claim 37 is drawn to a computer running a computer program, the computer program executing instructions for performing a method comprising:

--receiving information relating to a monoatomic metal ion to be simulated;

--and generating, for observation by a user on a display, a representation of the monoatomic metal ion as a metal molecule by a molecular dynamics simulation, wherein said metal molecule comprises a plurality of atoms comprising a center atom and one or more dummy atoms, wherein said center atom has a van der Waals radius greater than zero and has a charge of zero, wherein said center atom is covalently linked to said one or more dummy atoms, and wherein each dummy atom has a positive charge.

Claim 55 is drawn to a computer readable computer program limited to perform the method executed by the machine in instant claim 37.

Clemmer et al. studies physical and chemical evidence for metallofullerenes as part of the cage. Specifically, Clemmer et al. studies carbon fullerene cages with between 28 and 50 carbons wherein the carbons are covalently bound to a niobium metal atom that is part of the cage. The niobium atom is the monoatomic metal ion, which, along with the carbon fullerene cage is interpreted to be the metal molecule. A carbon atom is considered to be the "center atom" with a charge of zero and a van der Waals radius greater than zero that is covalently bound to the niobium "niobium" atom with positive charge. It is inherent that niobium as an ion has a positive charge as shown on the 'Niobium' web page. It is also inherent that fullerene cages have a neutral (charge of zero) charge and a non-zero radius as taught in the title of Schlatholter et al.

However, Clemmer et al. does not demonstrate the computerized limitations (i.e. a computer simulation of the metal ion on a computer) limitations of the instant set of claims.

The article of Stote et al. studies zinc binding to proteins and solution. The acknowledgements section on page 29 of Stote et al. teaches use of CRAY, SGI, and SUN workstations to process the molecular dynamics simulations of zinc binding to proteins.

With regard to claims 38-39 and 56-57, the dummy atom niobium in Clemmer et al. has a mass of about or greater than about 0.1 g/mol.

With regard to claims 40-41 and 58-59, the carbon fullerenes of Clemmer et al. are polyhedrons wherein the dummy atom of niobium is at the apices of the polyhedron and the center atom carbon is in the center of the polyhedron.

With regard to claims 44 and 62, the metal ion is the transition metal niobium.

With regard to claims 45-47 and 63-65, Stote et al. simulates zinc (see title and abstract).

With regard to claims 52-54 and 70-72, the niobium in Clemmer et al. has a charge of about +.5, +.3333, and between about 0.1 and about +3 (i.e. see 'Niobium' web page)



It would have been obvious to someone of ordinary skill in the art at the time of the instant invention to modify the of niobium doped fullerene molecules of Clemmer et al. by use of the modeling of a metal using advanced computer systems as taught by Stote et al. wherein the motivation would have been that the computer apparatus of Stote et al. have the advantage of fast, and accurate simulation [i.e. see Acknowledgements on page 29 of Stote et al.] It would have been further obvious to substitute the zinc in Stote et al. for the niobium in Clemmer et al. to yield the predictable result of an alternate method of simulating carbide complexes. There would have been a reasonable expectation of success in substituting zinc for niobium because they are both transition elements with analogous properties in *in silico* molecular dynamics simulations.

Response to arguments:

Applicant's arguments with respect to the instant claims have been considered but are moot in view of the new ground(s) of rejection.

The following rejection is newly applied and necessitated by applicant's amendments:

35 U.S.C. 103 Rejection #2:

Claims 42-43 and 60-61 are rejected under 35 U.S.C. 103(a) as being unpatentable over Clemmer et al. as evidenced by 'Niobium' as evidenced by Schlatholter et al. in view of Stote et al. as applied to claims 37-41, 44-47, 52-59, 62-65,

and 68-72 above, and further in view of Barnett et al. [J. Cryst. Mol. Struct, 1972, volume 2, pages 271-279].

Claims 42-43 and 60-61 are further limiting wherein the polyhedron shape comprises a tetrahedron.

Clemmer et al. and Stote et al. make obvious a computerized method for simulating metal ions, as discussed above.

Clemmer et al. and Stote et al. do not demonstrate a metal ion in a tetrahedral complex.

The article of Barnett et al. studies the crystal and molecular structure of tricyclohexylphosphineethylenenickel tricarbonyl. The abstract and the schematic on page 272 of Barnett et al. illustrates a tetrahedral structure of the nickel atom bound to four carbon atoms.

It would have been obvious to someone of ordinary skill in the art at the time of the instant invention to modify the zinc and niobium metal ion simulation methods of Clemmer et al. and Stote et al. by use of the tetrahedral structure of Barnett et al. because it is obvious to substitute known elements in the prior art to yield a predictable result. In this instance, the tetrahedral geometry in Barnett et al. is an alternate geometry than the fullerene geometries in Clemmer et al. There would have been a reasonable expectation of success in combining Clemmer et al., Stote et al. and Barnett et al. because the simulations of Stote et al. are generally applicable to the fullerene representations in Clemmer et al. as well as the tetrahedrons of Barnett et al.

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Response to Arguments

Applicant's additional arguments with respect to the instant claims have been considered but are moot in view of the new ground(s) of rejection.

The following rejection is newly applied and necessitated by applicant's amendments:

35 U.S.C. 103 Rejection #3:

Claims 48-51 and 66-69 are rejected under 35 U.S.C. 103(a) as being unpatentable over Clemmer et al. as evidenced by 'Niobium' as evidenced by Schlatholter et al. in view of Stote et al. as applied to claims 37-41, 44-47, 52-59, 62-65, and 68-72 above, and further in view of Aqvist et al. [Journal of the American Chemical Society, 1990, volume 112, pages 2860-2868; on IDS].

Claims 48 and 66 further limit the metal to be magnesium.

Claims 49 and 67 further limit the metal to be calcium.

Claims 50 and 68 are further limiting wherein the metal has a calculated energy of solvation about equal to an experimentally determined energy of solvation for the metal.

Claims 51 and 69 are further limiting wherein the calculated energy of solvation is within about 10% of said experimentally determined energy of solvation for said metal ion.

Clemmer et al. and Stote et al. make obvious a computerized method for simulating metal ions, as discussed above.

Clemmer et al. and Stote et al. do not simulate magnesium and calcium. Additionally, Andriotis et al. and Stote et al. do not find energies of solvation.

Aqvist et al. studies free energy relationships in metalloenzyme-catalyzed reactions.

Specifically, Figure 3 of Aquvist et al. compares calculated energies of solvation of calcium and magnesium with observed values.

It would have been obvious to someone of ordinary skill in the art at the time of the instant invention to modify the zinc and niobium metal ion simulation methods of Clemmer et al. and Stote et al. by use of the calcium and magnesium in Aquvist et al. because it is obvious to substitute known elements in the prior art to yield a predictable result. In this instance, calcium and magnesium are alternate metal ions for simulation as nickel and zinc. There would have been a reasonable expectation of success in combining Clemmer et al., Stote et al. and Aquvist et al. because all of the ions discussed are metals with analogous properties in *in silico* molecular dynamics simulations. It would have been further obvious to apply the simulated energies of solvation of Aquvist et al. to the simulations of Clemmer et al. and Stote et al. because Aquvist et al. presents calculated energetics in agreement with experimental data (i.e. see Figure 3 of Aquvist et al.).

#### Response to Arguments

Applicant's additional arguments with respect to the instant claims have been considered but are moot in view of the new ground(s) of rejection.

***Conclusion***

No claim is allowed.

Applicant's amendment necessitated the new ground(s) of rejection presented in this Office action. Accordingly, **THIS ACTION IS MADE FINAL**. See MPEP § 706.07(a). Applicant is reminded of the extension of time policy as set forth in 37 CFR 1.136(a).

A shortened statutory period for reply to this final action is set to expire THREE MONTHS from the mailing date of this action. In the event a first reply is filed within TWO MONTHS of the mailing date of this final action and the advisory action is not mailed until after the end of the THREE-MONTH shortened statutory period, then the shortened statutory period will expire on the date the advisory action is mailed, and any extension fee pursuant to 37 CFR 1.136(a) will be calculated from the mailing date of the advisory action. In no event, however, will the statutory period for reply expire later than SIX MONTHS from the date of this final action.

Papers related to this application may be submitted to Technical Center 1600 by facsimile transmission. Papers should be faxed to Technical Center 1600 via the central PTO Fax Center. The faxing of such pages must conform with the notices published in the Official Gazette, 1096 OG 30 (November 15, 1988), 1156 OG 61 (November 16, 1993), and 1157 OG 94 (December 28, 1993)(See 37 CFR § 1.6(d)). The Central PTO Fax Center Number is (571) 273-8300.

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Any inquiry concerning this communication or earlier communications from the examiner should be directed to Russell Negin, whose telephone number is (571) 272-1083. The examiner can normally be reached on Monday-Friday from 7am to 4pm.

If attempts to reach the examiner by telephone are unsuccessful, the examiner's Supervisor, Marjorie Moran, Supervisory Patent Examiner, can be reached at (571) 272-0720.

Information regarding the status of the application may be obtained from the Patent Application Information Retrieval (PAIR) system. Status information for published applications may be obtained from either Private PAIR or Public PAIR. Status information for unpublished applications is available through Private PAIR only. For more information on the PAIR system, contact the Electronic Business Center (EBC) at 866-217-9197 (toll-free).

/RSN/  
Russell S. Negin  
1 June 2009

/Marjorie Moran/  
Supervisory Patent Examiner, Art Unit 1631